

Software for processing high-data-rate MX in CIF and NeXus/HDF5

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As the rate of production of diffraction images rises to several hundred datasets per day per beamline, it is becoming increasingly important to record images and metadata in an efficiently-retrievable form. As data rates increase further it will become impractical to handle the same images multiple times in order to transform images from one convention to another. The last time our community faced a similar speed-constrained transition was with the Dectris Pilatus pixel-array detectors which strained computers and networks of that time by producing ten images per second, leading to the adoption of the imgCIF/CBF and miniCBF metadata conventions. Now, with data arriving one to three orders of magnitude faster, the introduction of NeXus/HDF5 images, and adoption of new experimental techniques including serial synchrotron crystallography, consistent well-documented crystallographic-image data and metadata handling is essential to conserve processing resources and maximize beamline structure production. To this end, the necessary concordances of imgCIF/CBF – miniCBF – NeXus NXmx metadata specifications [1] [2] [3] are being maintained on a common web site, with links to supporting software packages. We review the current status of these efforts and discuss the implications for software developers and crystallographers.

[1] H. J. Bernstein, J. M. Sloan, G. Winter, T. S. Richter, NIAC, COMCIFS, "Coping with BIG DATA image formats: integration of CBF, NeXus and HDF5", Computational Crystallography Newsletter, 2014, 5, 12 – 18.

[2] A. S. Brewster, J. Hattne, J. M. Parkhurst, D. G. Waterman, H. J. Bernstein, G. Winter, N. K. Sauter, "XFEL Detectors and ImageCIF", Computational Crystallography Newsletter, 2014, 5, 19 – 25.

[3] M. Mueller, "EIGER HDF5 data and NeXus format", in Workshop on Metadata for raw data from X-ray diffraction and other structural techniques, 22 – 23 Aug 2015, Rovinj, Croatia.

Work supported in part by Dectris.



Keywords: [CIF](#), [NeXus](#), [Eiger](#)